About saddle point approximation:

We want to approximate the following integral

$$I = \int_a^b dx\, e^{N\phi(x)}$$

where $\phi(x)$ has a maximum in $x_0 \in [a,b]$

and $\phi(x) \underset{N\to\infty}{\sim} O(1)$ all the dependence in N has been factorized!

$$I = \int_a^b dx\, e^{N\left[\phi(x_0) + \cancel{(x-x_0)\phi'(x_0)} + \frac{1}{2}(x-x_0)^2 \overset{<0}{\phi''(x_0)} + \sum_{m\geq 3} \frac{(x-x_0)^m}{m!}\phi\Big|_{x_0}\right]}$$

Taylor expansion around the maximum

$$= e^{N\phi(x_0)} \int_a^b dx\, e^{-\frac{N}{2}(x-x_0)^2|\phi''(x_0)| + N\sum_{m\geq 3}\frac{(x-x_0)^m}{m!}\phi^{(k)}\Big|_{x_0}}$$

also I can extend the limit of integration

$$= e^{N\phi(x_0)} \underbrace{\int_{-\infty}^{+\infty} dx\, e^{-\frac{N}{2}(x-x_0)^2|\phi''(x_0)|}}_{\text{gaussian distribution, upon normalization...}} e^{Nu} \quad \text{with } u = \sum_{m\geq 3}\frac{(x-x_0)^m}{m!}\phi^{(m)}\Big|_{x_0}$$

$$= e^{N\phi(x_0)} \sqrt{\frac{2\pi}{N|\phi''(x_0)|}} \int_{-\infty}^{+\infty} dx\, \sqrt{\frac{N|\phi''(x_0)|}{2\pi}}\, e^{-\frac{N(x-x_0)^2}{2}|\phi''(x_0)|} \sum_{k=0}^{\infty}\frac{N^k u^k}{k!}$$

$e^x = \sum_k \frac{x^k}{k!}$

$$= e^{N\phi(x_0)} \sqrt{\frac{2\pi}{N|\phi''(x_0)|}} \left\langle \sum_{k=0}^{\infty} \frac{N^k}{k!} u^k \right\rangle$$

with respect to $\rho(x) = \mathcal{N}\left(x_0, \frac{1}{N|\phi''(x_0)|}\right)$

$$= e^{N\phi(x_0)} \sqrt{\frac{2\pi}{N|\phi''(x_0)|}} \left[1 + N\langle u\rangle + \frac{N^2}{2}\langle u^2\rangle + \frac{N^3}{6}\langle \dots \rangle\right]$$

$$= e^{N\phi_0}\sqrt{\frac{2\pi}{N|\phi''(x_0)|}}\left[1 + N\sum_{m>2}\frac{\phi^{(m)}(x_0)}{m!}\underbrace{\langle (x-x_0)^m\rangle}_{\text{m- central moment of the Gaussian}} + \frac{N^2}{2}\sum_{\substack{m_1>2\\ m_2>2}}\frac{\phi^{(m_1)}(x_0)\,\phi^{(m_2)}(x_0)}{m_1!\,m_2!}\langle (x-x_0)^{m_1+m_2}\rangle + \frac{N^3}{6}\langle \dots \rangle + \dots\right]$$

Each of the term is of the form:

$$\underline{N^k \langle (x-x_0)^m\rangle \text{ with } m > 2k}$$

We can use <u>Wick's theorem</u>:

$$\langle (x-\mu)^m\rangle = \begin{cases} 0 & \text{if } m \text{ is odd} \\ a_m\,\sigma^m & \text{if } m \text{ is even} \end{cases}$$

where σ^2 is the variance

$$\boxed{\begin{array}{l}\langle x\rangle = \mu \\ \mathrm{var}(x) = \sigma^2\end{array}}$$

and $a_m = \frac{m!}{2^{m/2}\,(m/2)!} = (m-1)!$, it is a combinatorial prefactor

$\Rightarrow$ if m is even

$$\sim N^k\left(\frac{1}{N|\phi''(x_0)|}\right)^{m/2} \simeq N^{\overbrace{k-m/2}^{<0}} \xrightarrow[N\to\infty]{} 0$$

$m > 2k$

$k=1$ $m=4$ $\sim N^{-1}$
$k=2$, $m=6$ $\sim N^{-1}$

Let's compute the first order correction:

$$N\frac{\phi^{(4)}(x_0)}{\cancel{4!}}\,\frac{\cancel{4!}}{2^2\,2!}\left(\frac{1}{N^2|\phi''(x_0)|^2}\right) \pm \frac{N^2}{2}\frac{\left(\phi^{(III)}(x_0)\right)^2}{\underset{6}{3!}\;\underset{6}{3!}}\;\frac{6!}{2^3\,\underset{6}{3!}}\left(\frac{1}{N^3(\phi''(x_0))^3}\right)$$

$$= \frac{1}{N}\left[\frac{\phi^{(4)}(x_0)}{8\,|\phi''(x_0)|^2} + \frac{5}{24}\frac{\phi^{(iii)}(x_0)^2}{|\phi''(x_0)|^2} \right] + O\left(\frac{1}{N}\right)$$

$$I = \int_a^b dx\, e^{N\phi(x)} \simeq e^{N\phi(x_0)} \sqrt{\frac{2\pi}{N|\phi''(x_0)|}}$$

Gaussian approximation
to simplify this integral

For example, we use it to compute $\Omega(E_1) = \int dE_1\, p(E_1)$ in the microcanonical ensemble.

But also, consider a probability distribution of the form:

$$p(x) \propto e^{+N\underbrace{f(x)}} \qquad \text{with } f(x) \underset{N\to\infty}{\sim} O(1)$$

$$\max f(x) = f(x^*)$$

$$f''(x^*) < 0$$

this function
is often called
rate function

$$\boxed{\text{for example } p(E_1) \propto e^{\frac{N}{k_B}\left[s_1(E_1) + s_2(E - E_1)\right]}}$$

Then, the integral

$$I = \int dx\, e^{+Nf(x)}$$ can be computed as we just saw using the saddle point approximation

i.e. the integral can be treated as a Gaussian integral with a width $\sim \frac{1}{\sqrt{N}}$. But can the distribution itself be treated as Gaussian? yes!

Consider any observable $G(x)$, and compute the expectation value:

$$\langle G(x) \rangle = \frac{1}{I} \int dx\, G(x) e^{N f(x)} \quad \text{with } I = \int dx\, e^{N f(x)}$$

Idea is to take the Taylor expansion of $G(x)$ around the maximum x^* of $f(x)$

$$= \frac{1}{I} \int dx \sum_{m=0}^{\infty} \frac{G^{(m)}(x^*)}{m!} (x - x^*)^m e^{N f(x)}$$

$$= \frac{1}{I} \sum_m \frac{G^{(m)}(x^*)}{m!} \int dx\, (x - x^*)^m \underbrace{e^{N f(x)}}_{\text{you Taylor expand this}}$$

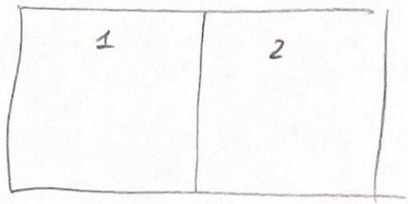
$$= \frac{e^{N f(x^*)}}{I} \sum_m \frac{G^{(m)}(x^*)}{m!} \int dx\, (x - x^*)^m \left(e^{-\frac{N}{2} |f''(x^*)| (x - x^*)^2} \right) e^{\sum_{l>2} N \frac{f^{(l)}(x^*)}{l!} (x - x^*)^l}$$

Same computation as before!

Conclusion:

Where did we use it in class?

For instance, in the microcanonical ensemble



$E = E_1 + E_2$

We <u>choose the macrostate</u>: in this case, we choose the macrostate of interest as being the energy of system 1.

$$P(E_1) = \sum_{E_2} \frac{\Omega_1(E_1) \times \Omega_2(E_2)}{\underbrace{\Omega(E)}_{\text{normalization}}} \delta_{E_1+E_2=E}$$

In general: macrostate e_n

$P(e_n) = \sum_{e_m \in e_n} P(e_m)$

it is a grouping!

$$= \frac{\Omega_1(E_1) \times \Omega_2(E-E_1)}{\Omega(E)}$$

where $\Omega(E) = \sum_{E_1} \Omega_1(E_1) \times \Omega_2(E-E_1)$ is the normalization

We take the continuum limit and use $S_m = k_B \ln \Omega(E)$

and the fact that S is <u>extensive in N</u>.

$$\Rightarrow \Omega(E) = \int dE_1 \, e^{\frac{N[s_1(E) + s_2(E-E_1)]}{k_B}}$$

zeroth law of thermodynamics

$$\Omega(E) \approx e^{\frac{N}{k_B}[s_1(E_1^*) + s_2(E-E_1^*)]} \quad \text{with} \quad \left.\frac{\partial S_1}{\partial E_1}\right|_{E_1^*} = \left.\frac{\partial S_2}{\partial E_2}\right|_{E_2^* = E - E^*}$$

Going back to the full $P(E_1)$

$$P(E_1) = e^{\frac{N}{k_B}\underbrace{\left[s_1(E_1) + s_2(E-E_1) - s_1(E_1^*) - s_2(E-E_2^*)\right]}_{\text{this is the "rate function"}}}$$

it is of the form that we discussed before!

$$\Rightarrow \boxed{P(E_1) \sim e^{\frac{-(E_1-E_1^*)^2}{2k_BT^2\left(\frac{C_V^1 C_V^2}{C_V^1+C_V^2}\right)}}}$$

What happens now if $2 \gg 1$? $C_V^2 \gg C_V^1$

2 = thermostat

1 = system = S

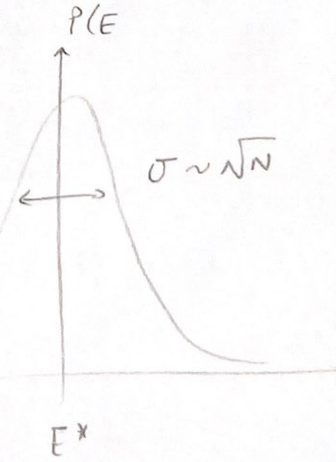
$$\Rightarrow P(E_S) \sim e^{\frac{-(E_1-E_1^*)^2}{2k_BT^2C_V}}$$

$\langle E_S \rangle = \langle E^* \rangle$ — the value that maximizes the rate function, which is the entropy in this case

$\sim N$ because the energy is extensive

$$C_V = \frac{\partial E}{\partial T} \sim N$$

$$\mathrm{var}(E_S) = C_V k_B T^2 \sim N$$



Typical fluctuations around the mean $\sim\sqrt{N}$ (still large!) but subextensive with respect to the value of the mean itself.

In the limit of $N \to \infty$, they are negligible!

This is why for macroscopic system, <u>thermodynamics works</u>! We have shown it from stat. mech. viewpoint

(it is an instance of the law of large number)

PROOF: a Gaussian distribution with $\sigma^2 \to \infty$ converges to a Dirac distribution

$$\lim_{\sigma^2 \to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-x_0)^2}{2\sigma^2}} = \delta(x-x_0)$$

Taylor expansion of $G(x)$

$$\langle G(x) \rangle = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} dx\, e^{-\frac{(x-x_0)^2}{2\sigma^2}} G(x) \overset{?}{=} G(x_0)$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} dx \sum_{k=0}^{N} \frac{G^{(k)}}{k!}\Big|_{x_0} (x-x_0)^k e^{-\frac{(x-x_0)^2}{2\sigma^2}} =$$

$$= \underbrace{G(x_0)}_{\text{happy}} + \sum_{k \geq 1} \frac{1}{k!} G^{(k)}\Big|_{x_0} \underbrace{\int_{-\infty}^{+\infty} \frac{(x-x_0)^k e^{-\frac{(x-x_0)^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}}}_{\langle (x-x_0)^k \rangle} =$$

$\langle (x-x_0)^k \rangle \to$ kth- centered moment of the Gaussian

$$\langle (x-x_0) \rangle = 0$$

$$\langle (x-x_0)^2 \rangle = \mathrm{var}(x) = \sigma^2 \to 0$$

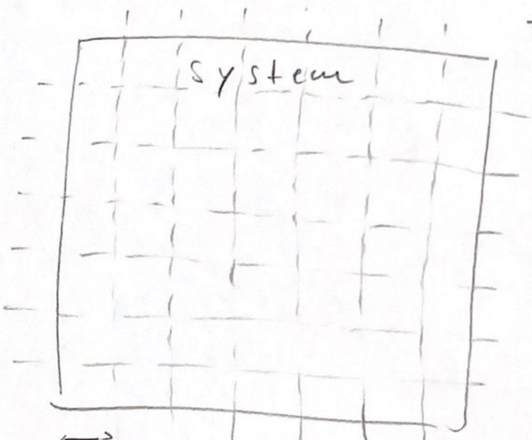
Wick's theorem:
$$\begin{cases} \langle (x-x_0)^k \rangle = 0 & \text{if } k \text{ is odd} \\ \langle (x-x_0)^k \rangle = a_k \underbrace{\sigma^k}_{(\sigma^2)^{k/2}} & \text{if } k \text{ is even} \end{cases}$$

All of the terms are either zero or $\sim \theta^k \xrightarrow[\theta \to 0]{} 0$.

$\square$

An alternative way to see it, is by using the <u>central limit theorem</u>

Very big system:



thermostat

$\ell \gg \xi$ correlation length

$\Rightarrow$ I can treat the subsystems as independent. (ask)

$E_{tot} \simeq \sum_{i=1}^{n} E_i$ where E_i is the energy of subsystem i

$p(E_{tot}) = ?$ as $n \to \infty$

E_{tot} is a sum of weakly correlated random variables.

Recalling from recitation on probability theory:

$Y = \sum_{i=1}^{N} x_i$ sum of i.i.d random variables

Introducing $y = \frac{1}{\sqrt{N}} (Y - \langle Y \rangle)$

$$\Rightarrow \boxed{\lim_{N\to\infty} P(y) = \frac{1}{\sqrt{2\pi\langle x^2\rangle_c}}\, e^{-\frac{y^2}{2\langle x^2\rangle_c}}}$$

statement of the central limit theorem

Characteristic function for y:

$$\varphi_y(k) = \langle e^{-iky}\rangle$$

Cumulant expansion:

$$\psi_y(k) = \ln \varphi_y(k) = \overbrace{\sum_{n=1}^{\infty} \frac{(-ik)^n}{n!}\langle y^n\rangle_c}^{\text{by definition of cumulants}}$$

what do we know about the cumulants:

$$\langle y\rangle_c = \langle y\rangle = 0 \quad \text{first}$$

$$\langle y^2\rangle_c = \frac{1}{N}\left\langle \left[\sum_{i=1}^{N}(x_i - \langle x_i\rangle)\right]^2\right\rangle$$

$$\langle y^l\rangle_c = \frac{1}{N^{l/2}}\left\langle \left[\sum_{i=1}^{N}(x_i - \langle x_i\rangle)\right]^l\right\rangle_c$$

now, because the variables $x_1, \dots, x_N$ are independent and identically distributed $P(x_1, \dots, x_N) = \prod_i P_i(x_i)$

$$\Rightarrow \varphi_y(k) = \prod_i \varphi_i(k)$$

$$\Rightarrow \psi_y(k) = \sum_i \psi_i(k)$$

$$\Rightarrow \left\langle \left[\sum_{i=1}^{N}(x_i - \langle x_i\rangle)\right]^n\right\rangle_c = \sum_{i=1}^{N}\langle (x_i - \langle x_i\rangle)^n\rangle_c$$

it becomes the sum of the individual cumulants

$$\Rightarrow \left\langle \left[\sum_{i=1}^{N} (x_i - \langle x_i \rangle) \right]^n \right\rangle_c = N \left\langle (x_i - \langle x_i \rangle)^n \right\rangle_c$$

$$\Rightarrow \langle y^l \rangle_c \sim N^{1 - l/2} \xrightarrow[N \to \infty]{} 0 \quad \forall \; \underline{\underline{l > 2}}$$

The Gaussian is indeed the only distribution with only the first two cumulants that are finite and the higher-order cumulants equal to zero.

Comments

- the CLT applies more generally also for weakly-correlated variables as long as their cross variances $\sum_{i_1, \dots i_m} \langle x_{i_1} x_{i_2} \dots x_{i_m} \rangle \ll O(N^{m/2})$.

- For the CLT to hold we assume $\langle X^2 \rangle_c < \infty$. If the distribution of the individual variables is for instance $p(x) \sim \frac{1}{|x|^{1+\alpha}}$ $\quad 0 < \alpha < 2$, the distribution is normalizable but $\langle x^2 \rangle_c = +\infty$.

Then, for $y = \frac{Y - \langle y \rangle}{N^{1/\alpha}}$ the distribution converges to a <u>Levy distribution</u>

ex. $\alpha = 1$ $\quad p(y) \sim \frac{a}{\pi (y^2 + a^2)}$ $\quad$ power law decay

NB The central limit theorem applies to $y \neq \sum_{i=1}^{N} x_i$

Actually since $y = \frac{1}{\sqrt{N}} \left(\sum_{i=1}^{N} x_i - \langle \sum_{i=1}^{N} x_i \rangle \right)$

$y \sim O(1) \Rightarrow \sum_{i=1}^{N} x_i - \langle \sum_{i=1}^{N} x_i \rangle \sim \sqrt{N}$

The sum of N i.i.d RV has fluctuations of order $\sim \sqrt{N}$. It is the case of the energy!

Connecting the CLT to the energy $E_{tot} = \sum_{i=1}^{n} E_i$

$$P(Y)\, dY = P(y)\, dy$$

$$P(Y) = P(y) \frac{dy}{dY} \qquad \text{where } y = \frac{(Y - \langle Y \rangle)}{\sqrt{N}}$$

$$\frac{1}{\sqrt{N}}$$

$$= \frac{1}{\sqrt{2\pi N \langle x^2 \rangle_c}} e^{-\frac{(Y - \langle Y \rangle)^2}{2N \langle x^2 \rangle_c}}$$

I call $\sigma_Y^2 = N \langle x^2 \rangle_c$

$$= \frac{1}{\sqrt{2\pi \sigma_Y^2}} e^{-\frac{1}{2} \frac{(Y - \langle Y \rangle)^2}{\sigma_Y^2}}$$

where now the N-dependence is hidden in $\sigma_Y^2 \sim N$

This is the result we obtained for $P(E_1)$!

NB When $N \to \infty$ the exponent vanish except when

$$\boxed{y - \langle y \rangle \sim \sqrt{N}}$$

Again, these are the fluctuations that we are capturing.

or when $y \to \langle y \rangle$, which is the <u>law of large numbers</u>.

Finally, Stirling approximation from saddle point method:

$$N! \simeq \left(\frac{N}{e}\right)^N \sqrt{2\pi N} = e^{N\ln N - N} \sqrt{2\pi N}$$

$$N! = \Gamma(N+1) = \int_0^\infty dx \; x^N e^{-x} = \int_0^\infty dx \; e^{N\ln x - x}$$

change of variable: $y = \frac{x}{N}$ $\quad dy = \frac{dx}{N}$

$$= N \int_0^\infty dy \; e^{N\ln Ny - Ny} = N \int_0^\infty dy \; e^{N(\ln y - y)} \, e^{N\ln N} =$$

$$= N e^{N\ln N} \int_0^\infty dy \; e^{N \underbrace{(\ln y - y)}_{f(y)}}$$

$f'(y) = \frac{1}{y} - 1 \implies y^* = 1$ maximum

$f''(y) = -\frac{1}{y^2} < 0$ it is a concave function! Good...

$$\Rightarrow N! \simeq N e^{N\ln N} \int_0^\infty dy\, e^{N\left[f(y^*) + \cancel{(y-y^*) f'(y^*)} + \frac{1}{2}(y-y^*)^2 \underbrace{f''(y^*)}_{-1} + \dots \right.}$$

$$\simeq N e^{N\ln N} e^{-N} \int_0^\infty dy\, e^{\frac{-N(y-1)^2}{2}} =$$

$\bar{y} = y-1$
expand extreme of integration

$$= N e^{N\ln N} e^{-N} \int_{-\infty}^{+\infty} d\bar{y}\, e^{\frac{-N\bar{y}^2}{2}} = N e^{N\ln N} e^{-N} \sqrt{\frac{2\pi}{N}}$$

$$= \sqrt{2\pi N}\; e^{N\ln N - N} + O\left(\frac{1}{N}\right)$$